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Dynamics of a polymer nanocomposite during active deformation ROBERT RIGGLEMAN, GREGORY TOEPPERWEIN, JUAN DE PABLO, HAU-NAN LEE, M. D. EDIGER, University of Wisconsin, Madison — Recent molecular simulation and experimental studies have explored the effects of stress on the dynamics of polymer glasses and both have demonstrated that relaxation times can decrease by more than two orders of magnitude. However, many questions on the origins of the changes in the dynamics remain unaddressed. In this study, we have performed extensive molecular dynamics and Monte Carlo simulations of a polymer glass and a polymer nanocomposite undergoing active deformation. We measure the dynamics during both constant stress and constant strain rate deformations and provide a detailed comparison of the two modes of deformation. The nanoparticles impart mechanical reinforcement onto the polymer, requiring larger stresses to achieve the same deformation. In both systems, the dynamics correlate very well with the instantaneous strain rate whether we deform at constant stress or constant strain rate. Additionally, we explore the effects of each mode of deformation on the potential energy landscape and find qualitatively different behaviors when we deform at constant stress versus constant strain rate. Finally, we provide a brief comparison of our simulation results to recent experiments and demonstrate that the simulations are capable of reproducing all of the behaviors observed in the experiments.

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